

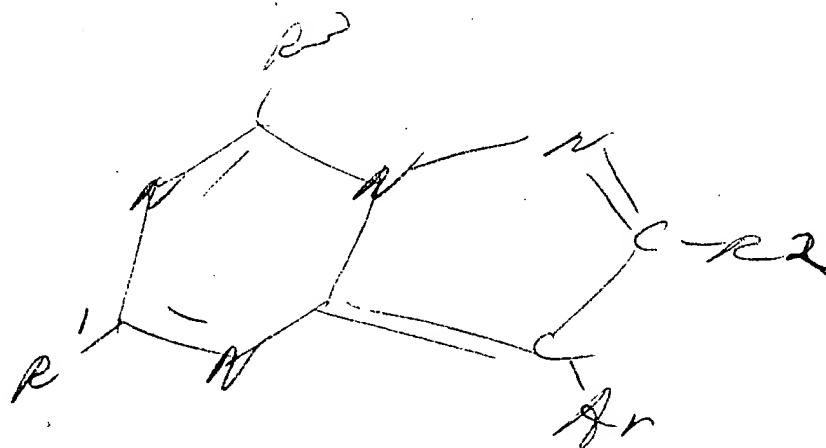
## ONLINE SEARCH REQUEST FORM

8-862

USER J. H. FordSERIAL NUMBER 09/315002ART UNIT 1644PHONE 382-4231DATE 2-26-744D09

Please give a detailed statement of requirements. Describe as specifically as possible the subject matter to be searched. Define any terms that may have special meaning. Give examples or relevant citations, authors, or keywords, if known.

You may include a copy of the broadest and or relevant claim(s).



431.74

8 18  
7 5 17 18

45125

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## STAFF USE ONLY

Call'd 9/2

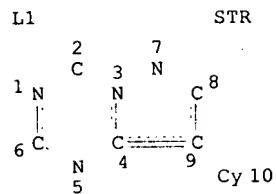
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- SDC
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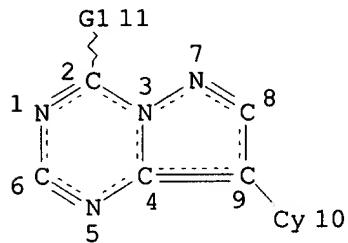
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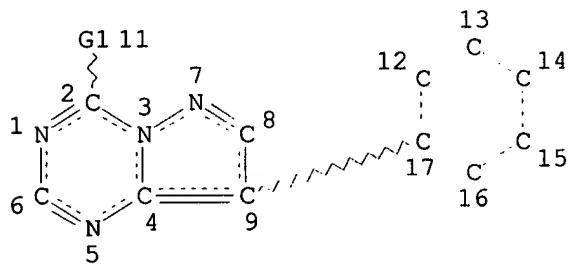
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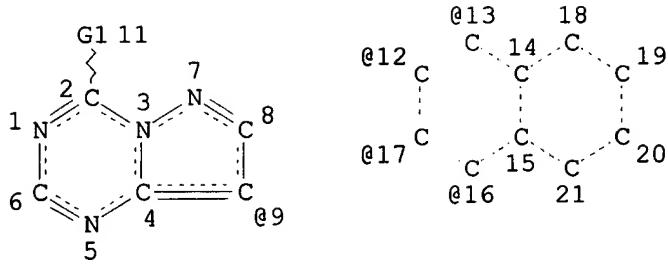
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VPA 9-13/12/17/16 U

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DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE

L9 1 SEA FILE=REGISTRY SUB=L7 SSS FUL L8

100.0% PROCESSED 1 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.04

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1998 ACS

RN 117414-30-9 REGISTRY

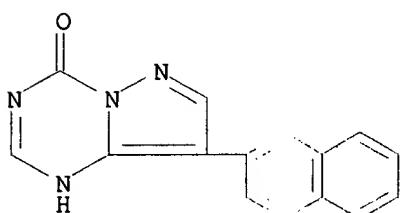
CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-(2-naphthalenyl)- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C15 H10 N4 O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

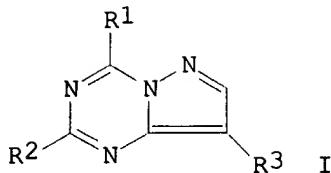


1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:211092 Preparation of pyrazolotriazines as xanthine oxidase inhibitors. Fujii, Setsuro; Kawamura, Hiroyuki; Kiyokawa, Hiroshi; Yamada, Satoshi (Otsuka Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP 269859 A2 880608, 141 pp. DESIGNATED STATES: R: CH, DE, ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 87-115806 871028. PRIORITY: JP 86-261008 861031; JP 87-73911 870326; JP 87-120688 870518; JP 87-159437 870625.

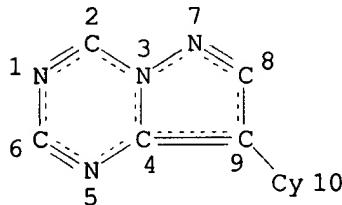
GI



AB The title compds. [I; R1 = OH, alkanoyloxy; R2 = H, OH, SH; R3 = naphthyl, (un)substituted Ph, heterocyclyl] were prep'd. PhCH2CN and HCO2Et were stirred 3 h in C6H6 contg. NaOMe to give PhCH(CHO)CN which was stirred 12 h with H2NCONHNH2.cndot.HCl in aq. MeOH to give 3-amino-2-carbamoyl-4-phenylpyrazole. The latter was stirred 13 h with HC(OEt)3 at 100-110.degree. to give I (R1 = OH, R2 = H, R3 = Ph). I [R1 = OH, R2 = H, R3 = 3,4-Me2Ph], at 5 mg/kg orally, lowered serum uric acid in mice 73.6%. Tablets were prep'd. from a formulation contg. I [R1 = OH, R2 = H, R3 = 4-(4-MeC6H4S)C6H4] 100, cellulose 40, starch 30, Mg stearate 2 g coated with hydroxypropyl methylcellulose 10, polyethylene glycol 6000 3, castor oil 40 and EtOH 40 g.

=> d l11 que stat;d 1-10 ide cbib abs

L1 STR



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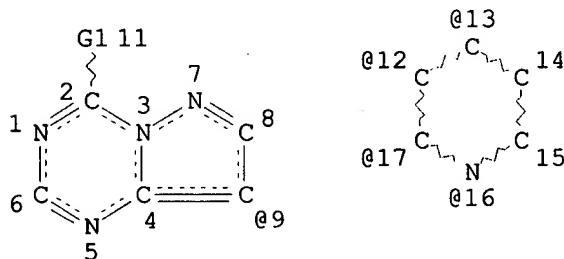
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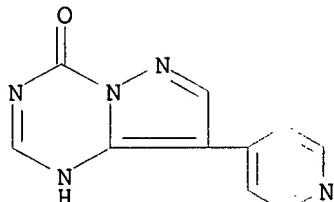
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STEREO ATTRIBUTES: NONE  
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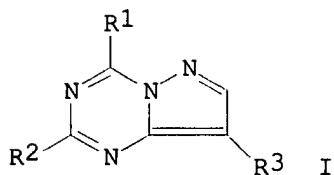
L11 ANSWER 1 OF 10 REGISTRY COPYRIGHT 1998 ACS  
RN 117414-24-1 REGISTRY  
CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-(4-pyridinyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C10 H7 N5 O  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:211092 Preparation of pyrazolotriazines as xanthine oxidase inhibitors. Fujii, Setsuro; Kawamura, Hiroyuki; Kiyokawa, Hiroshi; Yamada, Satoshi (Otsuka Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP 269859 A2 880608, 141 pp. DESIGNATED STATES: R: CH, DE, ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW.  
APPLICATION: EP 87-115806 871028. PRIORITY: JP 86-261008 861031; JP 87-73911 870326; JP 87-120688 870518; JP 87-159437 870625.

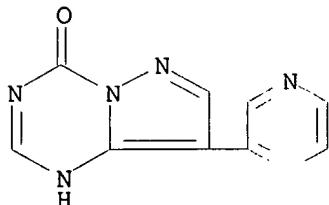
GI



AB The title compds. [I; R1 = OH, alkanoyloxy; R2 = H, OH, SH; R3 = naphthyl, (un)substituted Ph, heterocyclyl] were prep'd. PhCH2CN and

HCO<sub>2</sub>Et were stirred 3 h in C<sub>6</sub>H<sub>6</sub> contg. NaOMe to give PhCH(CHO)CN which was stirred 12 h with H<sub>2</sub>NCONHNH<sub>2</sub>.cntdot.HCl in aq. MeOH to give 3-amino-2-carbamoyl-4-phenylpyrazole. The latter was stirred 13 h with HC(OEt)<sub>3</sub> at 100-110.degree. to give I (R<sub>1</sub> = OH, R<sub>2</sub> = H, R<sub>3</sub> = Ph). I [R<sub>1</sub> = OH, R<sub>2</sub> = H, R<sub>3</sub> = 3,4-Me(PhSO)C<sub>6</sub>H<sub>3</sub>], at 5 mg/kg orally, lowered serum uric acid in mice 73.6%. Tablets were prep'd. from a formulation contg. I [R<sub>1</sub> = OH, R<sub>2</sub> = H, R<sub>3</sub> = 4-(4-MeC<sub>6</sub>H<sub>4</sub>S)C<sub>6</sub>H<sub>4</sub>] 100, cellulose 40, starch 30, Mg stearate 2 g coated with hydroxypropyl methylcellulose 10, polyethylene glycol 6000 3, castor oil 40 and EtOH 40 g.

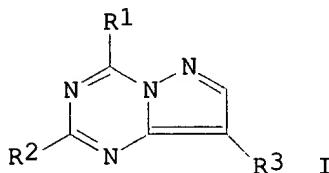
L11 ANSWER 2 OF 10 REGISTRY COPYRIGHT 1998 ACS  
 RN 117414-23-0 REGISTRY  
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 FS 3D CONCORD  
 MF C<sub>10</sub> H<sub>7</sub> N<sub>5</sub> O  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:211092 Preparation of pyrazolotriazines as xanthine oxidase inhibitors. Fujii, Setsuro; Kawamura, Hiroyuki; Kiyokawa, Hiroshi; Yamada, Satoshi (Otsuka Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP 269859 A2 880608, 141 pp. DESIGNATED STATES: R: CH, DE, ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW.  
 APPLICATION: EP 87-115806 871028. PRIORITY: JP 86-261008 861031; JP 87-73911 870326; JP 87-120688 870518; JP 87-159437 870625.

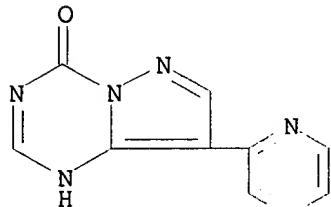
GI



AB The title compds. [I; R<sub>1</sub> = OH, alkanoyloxy; R<sub>2</sub> = H, OH, SH; R<sub>3</sub> = naphthyl, (un)substituted Ph, heterocyclyl] were prep'd. PhCH<sub>2</sub>CN and HCO<sub>2</sub>Et were stirred 3 h in C<sub>6</sub>H<sub>6</sub> contg. NaOMe to give PhCH(CHO)CN which was stirred 12 h with H<sub>2</sub>NCONHNH<sub>2</sub>.cntdot.HCl in aq. MeOH to give 3-amino-2-carbamoyl-4-phenylpyrazole. The latter was stirred 13 h with HC(OEt)<sub>3</sub> at 100-110.degree. to give I (R<sub>1</sub> = OH, R<sub>2</sub> = H, R<sub>3</sub> = Ph). I [R<sub>1</sub> = OH, R<sub>2</sub> = H, R<sub>3</sub> = 3,4-Me(PhSO)C<sub>6</sub>H<sub>3</sub>], at 5 mg/kg orally, lowered serum uric acid in mice 73.6%. Tablets were prep'd.

from a formulation contg. I [R1 = OH, R2 = H, R3 = 4-(4-MeC6H4S)C6H4] 100, cellulose 40, starch 30, Mg stearate 2 g coated with hydroxypropyl methylcellulose 10, polyethylene glycol 6000 3, castor oil 40 and EtOH 40 g.

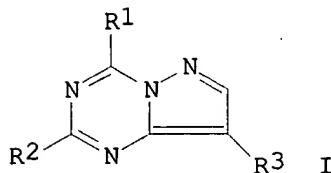
L11 ANSWER 3 OF 10 REGISTRY COPYRIGHT 1998 ACS  
 RN 117414-22-9 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-(2-pyridinyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C10 H7 N5 O  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:211092 Preparation of pyrazolotriazines as xanthine oxidase inhibitors. Fujii, Setsuro; Kawamura, Hiroyuki; Kiyokawa, Hiroshi; Yamada, Satoshi (Otsuka Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP 269859 A2 880608, 141 pp. DESIGNATED STATES: R: CH, DE, ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 87-115806 871028. PRIORITY: JP 86-261008 861031; JP 87-73911 870326; JP 87-120688 870518; JP 87-159437 870625.

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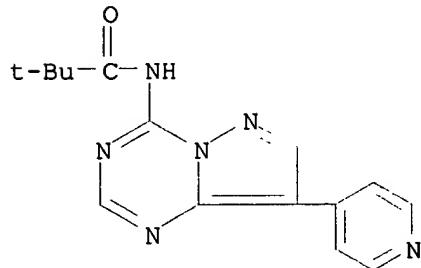
AB The title compds. [I; R1 = OH, alkanoyloxy; R2 = H, OH, SH; R3 = naphthyl, (un)substituted Ph, heterocyclyl] were prep'd. PhCH2CN and HCO2Et were stirred 3 h in C6H6 contg. NaOMe to give PhCH(CHO)CN which was stirred 12 h with H2NCONHNH2.cntdot.HCl in aq. MeOH to give 3-amino-2-carbamoyl-4-phenylpyrazole. The latter was stirred 13 h with HC(OEt)3 at 100-110.degree. to give I (R1 = OH, R2 = H, R3 = Ph). I [R1 = OH, R2 = H, R3 = 3,4-Me(PhSO)C6H3], at 5 mg/kg orally, lowered serum uric acid in mice 73.6%. Tablets were prep'd. from a formulation contg. I [R1 = OH, R2 = H, R3 = 4-(4-MeC6H4S)C6H4] 100, cellulose 40, starch 30, Mg stearate 2 g coated with hydroxypropyl methylcellulose 10, polyethylene glycol 6000 3, castor oil 40 and EtOH 40 g.

L11 ANSWER 4 OF 10 REGISTRY COPYRIGHT 1998 ACS

RN 61959-48-6 REGISTRY  
 CN Propanoic acid, 2,2-dimethyl-, compd. with 2,2-dimethyl-N-[8-(4-pyridinyl)pyrazolo[1,5-a]-1,3,5-triazin-4-yl]propanamide (1:1) (9CI)  
 (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Propanamide, 2,2-dimethyl-N-[8-(4-pyridinyl)pyrazolo[1,5-a]-1,3,5-triazin-4-yl]-, mono(2,2-dimethylpropanoate) (9CI)  
 CN Pyrazolo[1,5-a]-1,3,5-triazine, propanamide deriv.  
 MF C15 H16 N6 O . C5 H10 O2  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

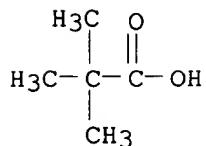
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CM 2

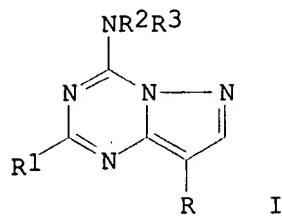
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1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney,  
 Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA).  
 U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
 APPLICATION: US 75-581388 750527.

GI



AB 4-Pyridomalonodialdehyde was treated with HONH<sub>2</sub> to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)<sub>3</sub> to give the pyrazolotriazine I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R<sub>1</sub>-R<sub>3</sub> = H; R = 4-pyridyl, R<sub>1</sub> = H, Me, R<sub>2</sub> = R<sub>3</sub> = Me) were similarly prep'd. I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H) was converted to I (R = 4-pyridyl; R<sub>1</sub> = R<sub>2</sub> = H; R<sub>3</sub> = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

L11 ANSWER 5 OF 10 REGISTRY COPYRIGHT 1998 ACS

RN 61959-47-5 REGISTRY

CN Propanamide, 2,2-dimethyl-N-[8-(4-pyridinyl)pyrazolo[1,5-a]-1,3,5-triazin-4-yl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyrazolo[1,5-a]-1,3,5-triazine, propanamide deriv.

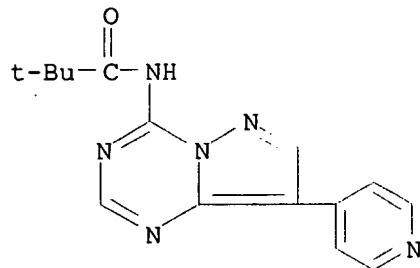
FS 3D CONCORD

MF C15 H16 N6 O

CI COM

LC STN Files: BEILSTEIN\*

(\*File contains numerically searchable property data)



L11 ANSWER 6 OF 10 REGISTRY COPYRIGHT 1998 ACS

RN 61959-46-4 REGISTRY

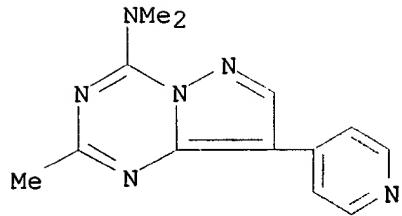
CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, N,N,2-trimethyl-8-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H14 N6

LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

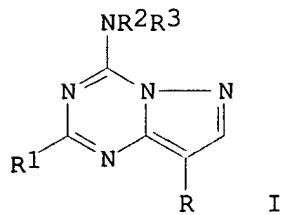
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1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

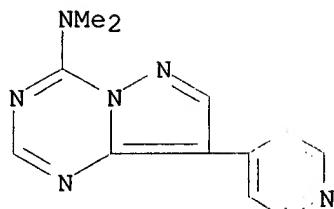
REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney, Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA). U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
 APPLICATION: US 75-581388 750527.

GI



AB 4-Pyridomalonaldehyde was treated with HONH<sub>2</sub> to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)<sub>3</sub> to give the pyrazolotriazine I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R<sub>1</sub>-R<sub>3</sub> = H; R = 4-pyridyl, R<sub>1</sub> = H, Me, R<sub>2</sub> = R<sub>3</sub> = Me) were similarly prep'd. I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H) was converted to I (R = 4-pyridyl; R<sub>1</sub> = R<sub>2</sub> = H; R<sub>3</sub> = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

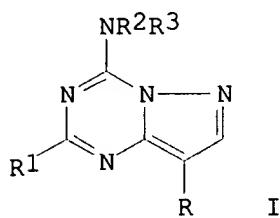
L11 ANSWER 7 OF 10 REGISTRY COPYRIGHT 1998 ACS  
 RN 61959-45-3 REGISTRY  
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 MF C12 H12 N6  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB,  
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1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

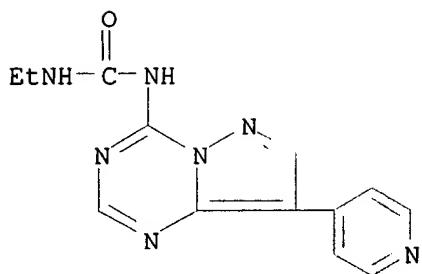
REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney, Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA). U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
 APPLICATION: US 75-581388 750527.

GI



AB 4-Pyridomalonalodialdehyde was treated with HONH2 to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)3 to give the pyrazolotriazine I (R = 4-pyridyl, R1-R3 = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R1-R3 = H; R = 4-pyridyl, R1 = H, Me, R2 = R3 = Me) were similarly prep'd. I (R = 4-pyridyl, R1-R3 = H) was converted to I (R = 4-pyridyl; R1 = R2 = H; R3 = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

L11 ANSWER 8 OF 10 REGISTRY COPYRIGHT 1998 ACS  
 RN 61959-43-1 REGISTRY  
 CN Urea, N-ethyl-N'-[8-(4-pyridinyl)pyrazolo[1,5-a]-1,3,5-triazin-4-yl]-, monohydrochloride (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Pyrazolo[1,5-a]-1,3,5-triazine, urea deriv.  
 MF C13 H13 N7 O . Cl H  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

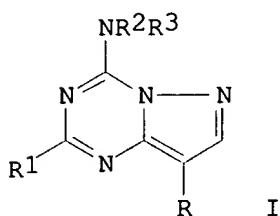


• HCl

1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney, Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA). U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
APPLICATION: US 75-581388 750527.

GI



AB 4-Pyridomalonaldehyde was treated with HONH<sub>2</sub> to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)<sub>3</sub> to give the pyrazolotriazine I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R<sub>1</sub>-R<sub>3</sub> = H; R = 4-pyridyl, R<sub>1</sub> = H, Me, R<sub>2</sub> = R<sub>3</sub> = Me) were similarly prep'd. I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H) was converted to I (R = 4-pyridyl; R<sub>1</sub> = R<sub>2</sub> = H; R<sub>3</sub> = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

L11 ANSWER 9 OF 10 REGISTRY COPYRIGHT 1998 ACS  
RN 61959-42-0 REGISTRY

CN Acetamide, N-[8-(4-pyridinyl)pyrazolo[1,5-a]-1,3,5-triazin-4-yl]-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

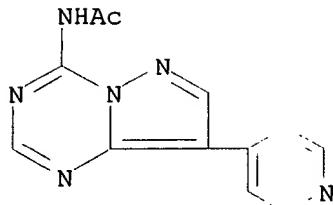
CN Pyrazolo[1,5-a]-1,3,5-triazine, acetamide deriv.

FS 3D CONCORD

MF C12 H10 N6 O

LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

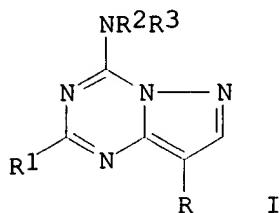
(\*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

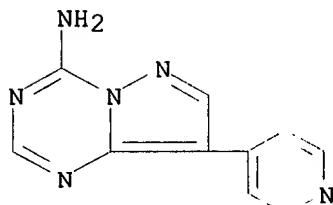
REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney, Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA). U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
 APPLICATION: US 75-581388 750527.

GI



AB 4-Pyridomalonaldehyde was treated with HONH<sub>2</sub> to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)<sub>3</sub> to give the pyrazolotriazine I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R<sub>1</sub>-R<sub>3</sub> = H; R = 4-pyridyl, R<sub>1</sub> = H, Me, R<sub>2</sub> = R<sub>3</sub> = Me) were similarly prep'd. I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H) was converted to I (R = 4-pyridyl; R<sub>1</sub> = R<sub>2</sub> = H; R<sub>3</sub> = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

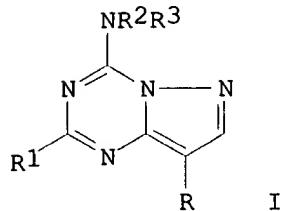
L11 ANSWER 10 OF 10 REGISTRY COPYRIGHT 1998 ACS  
 RN 61959-36-2 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, 8-(4-pyridinyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C10 H8 N6  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB,  
 USPATFULL  
 (\*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney,  
Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA).  
U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
APPLICATION: US 75-581388 750527.

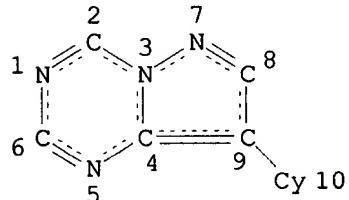
GI



AB 4-Pyridomalonaldehyde was treated with HONH<sub>2</sub> to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)<sub>3</sub> to give the pyrazolotriazine I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R<sub>1</sub>-R<sub>3</sub> = H; R = 4-pyridyl, R<sub>1</sub> = H, Me, R<sub>2</sub> = R<sub>3</sub> = Me) were similarly prep'd. I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H) was converted to I (R = 4-pyridyl; R<sub>1</sub> = R<sub>2</sub> = H; R<sub>3</sub> = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

=> d 113 que stat;d ide cbib abs

L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

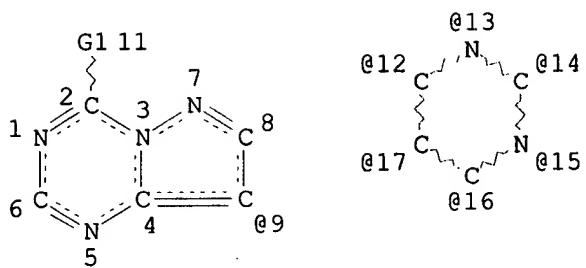
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NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L3 433 SEA FILE=REGISTRY SSS FUL L1

L12 STR



VAR G1=N/O  
VPA 9-17/12/13/16/14/15 U

NODE ATTRIBUTES:

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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
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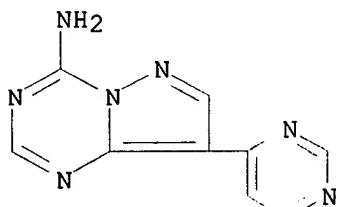
STEREO ATTRIBUTES: NONE

L13 1 SEA FILE=REGISTRY SUB=L3 SSS FUL L12

100.0% PROCESSED 5 ITERATIONS  
SEARCH TIME: 00.00.01

1 ANSWERS

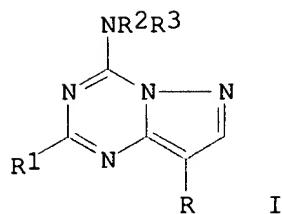
L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1998 ACS  
RN 62084-25-7 REGISTRY  
CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, 8-(4-pyrimidinyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C9 H7 N7  
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:106664 Pyrazolo [1,5-a] [1,3,5] triazines. Rooney, Clarence S.; Williams, Haydn Windsor R. (Merck and Co., Inc., USA). U.S. US 3995039 761130, 5 pp. (English). CODEN: USXXAM.  
APPLICATION: US 75-581388 750527.

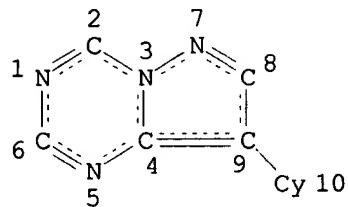
GI



AB 4-Pyridomalonodialdehyde was treated with HONH<sub>2</sub> to give 1-amidino-4-(4-pyridyl)-5-aminopyrazole which was cyclized with HC(OEt)<sub>3</sub> to give the pyrazolotriazine I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H). I (R = 4-pyrimidinyl, 2-pyrazinyl, R<sub>1</sub>-R<sub>3</sub> = H; R = 4-pyridyl, R<sub>1</sub> = H, Me, R<sub>2</sub> = R<sub>3</sub> = Me) were similarly prepd. I (R = 4-pyridyl, R<sub>1</sub>-R<sub>3</sub> = H) was converted to I (R = 4-pyridyl; R<sub>1</sub> = R<sub>2</sub> = H; R<sub>3</sub> = Ac, MeNHCO). At 5-25 mg I were bronchodilators.

=> d 115 que stat

L1 STR



## NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

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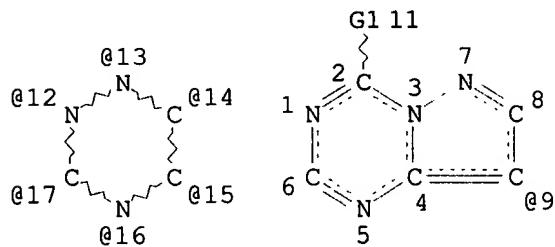
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NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L3 433 SEA FILE=REGISTRY SSS FUL L1

L14 STR



VAR G1=N/O  
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DEFAULT ECLEVEL IS LIMITED

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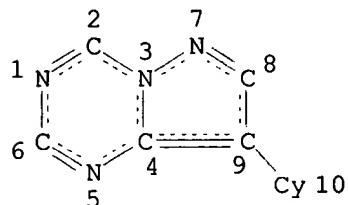
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NUMBER OF NODES IS 16

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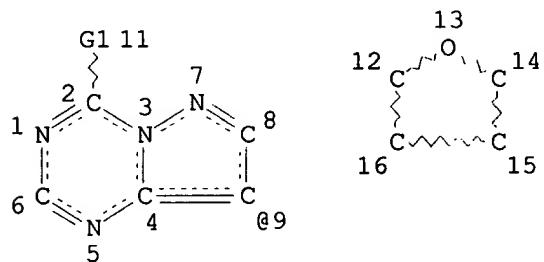
L1 STR



NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE  
L3 433 SEA FILE=REGISTRY SSS FUL L1  
L16 STR



VAR G1=N/O  
VPA 9-12/16/13 U  
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DEFAULT ECLEVEL IS LIMITED

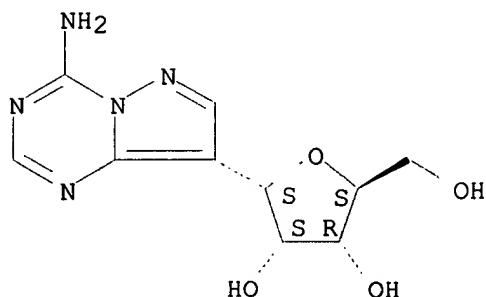
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NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE  
L17 37 SEA FILE=REGISTRY SUB=L3 SSS FUL L16

100.0% PROCESSED 275 ITERATIONS 37 ANSWERS  
SEARCH TIME: 00.00.02

L17 ANSWER 1 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 196086-00-7 REGISTRY  
 CN D-Ribitol, 5-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-2,5-anhydro-, (5S)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H13 N5 O4  
 SR CA  
 LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).

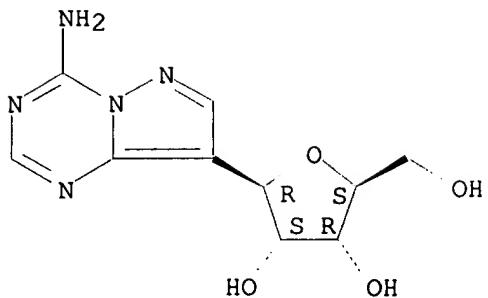


1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:262975 Synthesis of L-ribofuranosyl C-nucleosides.  
 Liang, Chengyi; Ma, Tianwei; Cooperwood, John S.; Du, Jinfa; Chu, Chung K. (Dep. Medicinal Chem., Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). Carbohydr. Res., 303(1), 33-38 (English) 1997.  
 CODEN: CRBRAT. ISSN: 0008-6215. Publisher: Elsevier.  
 AB C-Nucleosides, 4-amino-8-(.beta.-L-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine and 4-amino-7-(.beta.-L-ribofuranosyl)-5H-pyrrolo[3,2-d]pyrimidine (L-9-deazaadenosine), were synthesized from the key intermediate, 3-dimethylamino-2-(2,3-O-isopropylidene-5-O-trityl-L-ribofuranosyl)acrylonitrile, which was prep'd. from L-xylose in 11 steps. The synthesized C-nucleosides showed no significant antiviral activity.

L17 ANSWER 2 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 196085-98-0 REGISTRY  
 CN D-Ribitol, 5-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-2,5-anhydro-, (5R)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H13 N5 O4  
 SR CA  
 LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).

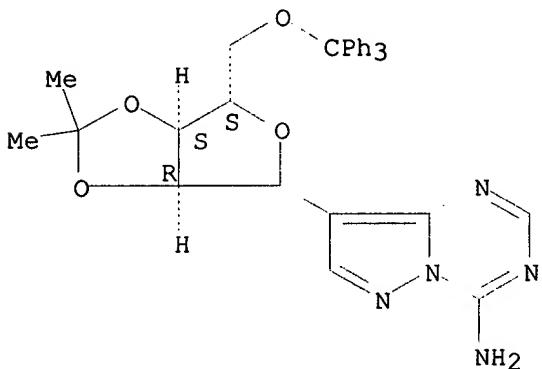


1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

- REFERENCE 1: 127:262975 Synthesis of L-ribofuranosyl C-nucleosides.  
 Liang, Chengyi; Ma, Tianwei; Cooperwood, John S.; Du, Jinfa; Chu, Chung K. (Dep. Medicinal Chem., Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). Carbohydr. Res., 303(1), 33-38 (English) 1997.  
 CODEN: CRBRAT. ISSN: 0008-6215. Publisher: Elsevier.
- AB C-Nucleosides, 4-amino-8-(.beta.-L-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine and 4-amino-7-(.beta.-L-ribofuranosyl)-5H-pyrrolo[3,2-d]pyrimidine (L-9-deazaadenosine), were synthesized from the key intermediate, 3-dimethylamino-2-(2,3-O-isopropylidene-5-O-trityl-L-ribofuranosyl)acrylonitrile, which was prep'd. from L-xylose in 11 steps. The synthesized C-nucleosides showed no significant antiviral activity.

L17 ANSWER 3 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 196085-96-8 REGISTRY  
 CN D-Ribitol, 5-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-2,5-anhydro-3,4-O-(1-methylethylidene)-1-O-(triphenylmethyl)-(9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C32 H31 N5 O4  
 SR CA  
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

- REFERENCE 1: 127:262975 Synthesis of L-ribofuranosyl C-nucleosides.

Liang, Chengyi; Ma, Tianwei; Cooperwood, John S.; Du, Jinfa; Chu, Chung K. (Dep. Medicinal Chem., Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). Carbohydr. Res., 303(1), 33-38 (English) 1997.

CODEN: CRBRAT. ISSN: 0008-6215. Publisher: Elsevier.

AB C-Nucleosides, 4-amino-8-(.beta.-L-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine and 4-amino-7-(.beta.-L-ribofuranosyl)-5H-pyrrolo[3,2-d]pyrimidine (L-9-deazaadenosine), were synthesized from the key intermediate, 3-dimethylamino-2-(2,3-O-isopropylidene-5-O-trityl-L-ribofuranosyl)acrylonitrile, which was prep'd. from L-xylose in 11 steps. The synthesized C-nucleosides showed no significant antiviral activity.

L17 ANSWER 4 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 185905-60-6 REGISTRY

CN 2-Furanmethanol, 5-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)tetrahydro-, (2S-trans)- (9CI) (CA INDEX NAME)

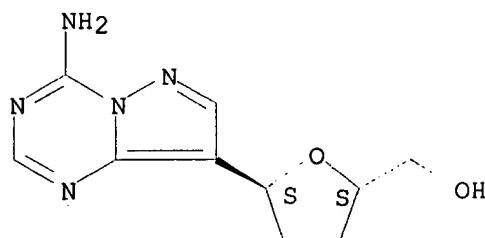
FS STEREOSEARCH

MF C10 H13 N5 O2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (-).



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:104355 Syntheses of 2',3'-dideoxy-D-C-nucleosides from .gamma.-lactone. Xiang, Yuejun; Du, Jinfa; Chu, Chung K. (Department of Medicinal Chemistry, College of Pharmacy, The University of Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(11 & 12), 1821-1834 (English) 1996. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Dekker.

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 2',3'-Dideoxy-D-C-nucleosides I, II, III, and IV have been synthesized from 2,3-dideoxy-D-glyceropentanoic acid .gamma.-lactone. These 2',3'-dideoxy-nucleosides were evaluated against HBV and HIV. No significant antiviral activities were found up to 100 .mu.M.

L17 ANSWER 5 OF 37 REGISTRY COPYRIGHT 1998 ACS

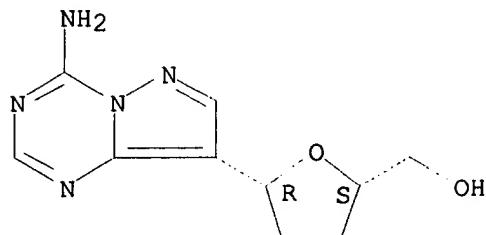
RN 185905-59-3 REGISTRY

CN 2-Furanmethanol, 5-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)tetrahydro-, (2S-cis)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H13 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:104355 Syntheses of 2',3'-dideoxy-D-C-nucleosides from .gamma.-lactone. Xiang, Yuejun; Du, Jinfa; Chu, Chung K. (Department of Medicinal Chemistry, College of Pharmacy, The University of Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(11 & 12), 1821-1834 (English) 1996. CODEN: NNUUD5. ISSN: 0732-8311. Publisher: Dekker.

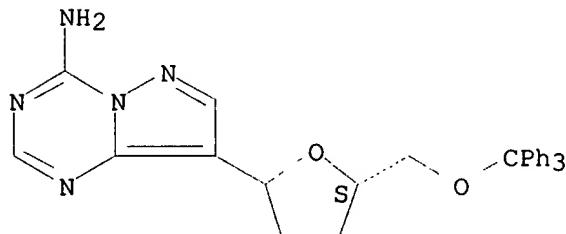
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 2',3'-Dideoxy-D-C-nucleosides I, II, III, and IV have been synthesized from 2,3-dideoxy-D-glyceropentanoic acid .gamma.-lactone. These 2',3'-dideoxy-nucleosides were evaluated against HBV and HIV. No significant antiviral activities were found up to 100 .mu.M.

L17 ANSWER 6 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 185905-58-2 REGISTRY  
CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, 8-[tetrahydro-5-[(triphenylmethoxy)methyl]-2-furanyl]-, (5S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H27 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:104355 Syntheses of 2',3'-dideoxy-D-C-nucleosides from .gamma.-lactone. Xiang, Yuejun; Du, Jinfa; Chu, Chung K. (Department of Medicinal Chemistry, College of Pharmacy, The University of Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(11 & 12), 1821-1834 (English) 1996. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Dekker.

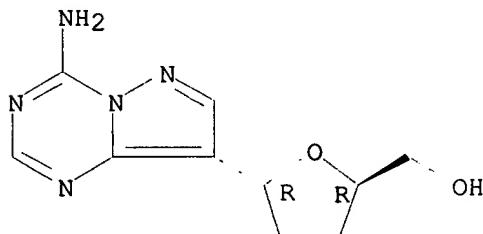
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 2',3'-Dideoxy-D-C-nucleosides I, II, III, and IV have been synthesized from 2,3-dideoxy-D-glyceropentanoic acid .gamma.-lactone. These 2',3'-dideoxy-nucleosides were evaluated against HBV and HIV. No significant antiviral activities were found up to 100 .mu.M.

L17 ANSWER 7 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 180062-02-6 REGISTRY  
CN 2-Furanmethanol, 5-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)tetrahydro-, (2R-trans)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C10 H13 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS

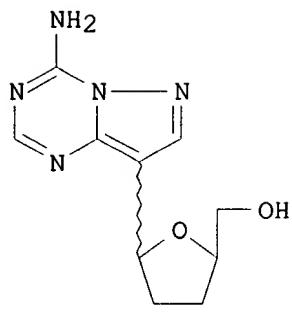
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:143192 Synthesis of 2',3'-dideoxy-L-glyceropentofuranosyl C-nucleosides. Lee, Chang Soo; Du, Jinfa; Chu, Chung K. (Dep. Med. Chem., Univ. Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(6), 1223-1236 (English) 1996. CODEN: NUNUD5. ISSN: 0732-8311.

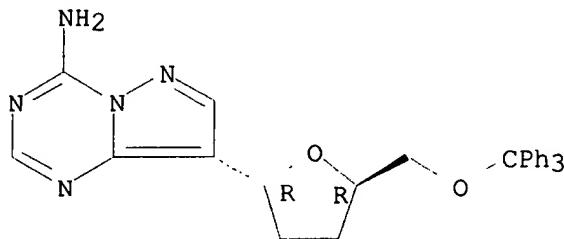
GI



AB 2',3'-Dideoxy-L-C-nucleosides, e.g. I, have been synthesized from L-gulonic .gamma.-lactone.

L17 ANSWER 8 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 180062-01-5 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, 8-[tetrahydro-5-[(triphenylmethoxy)methyl]-2-furanyl]-, (2R-trans)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C29 H27 N5 O2  
 SR CA  
 LC STN Files: CA, CAPLUS

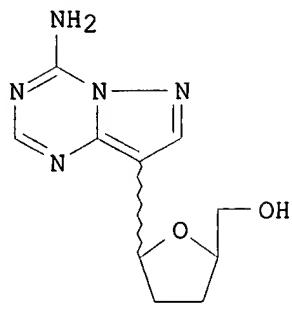
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:143192 Synthesis of 2',3'-dideoxy-L-glyceropentofuranosyl C-nucleosides. Lee, Chang Soo; Du, Jinfa; Chu, Chung K. (Dep. Med. Chem., Univ. Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(6), 1223-1236 (English) 1996.  
 CODEN: NUNUD5. ISSN: 0732-8311.

GI



AB 2',3'-Dideoxy-L-C-nucleosides, e.g. I, have been synthesized from L-gulonic .gamma.-lactone.

L17 ANSWER 9 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 179929-58-9 REGISTRY

CN 2-Furanmethanol, 5-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)tetrahydro-, (2R-cis)- (9CI) (CA INDEX NAME)

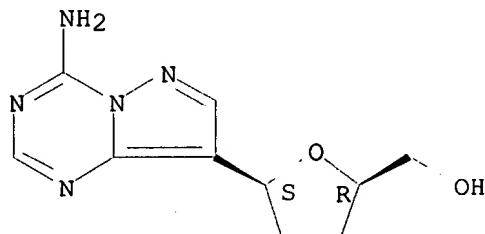
FS STEREOSEARCH

MF C10 H13 N5 O2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (-).

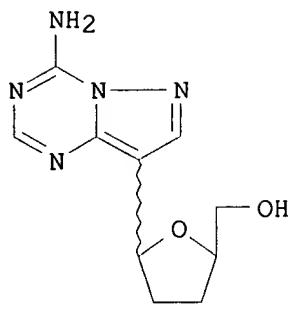


1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:143192 Synthesis of 2',3'-dideoxy-L-glyceropentofuranosyl C-nucleosides. Lee, Chang Soo; Du, Jinfa; Chu, Chung K. (Dep. Med. Chem., Univ. Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(6), 1223-1236 (English) 1996.  
CODEN: NNUUD5. ISSN: 0732-8311.

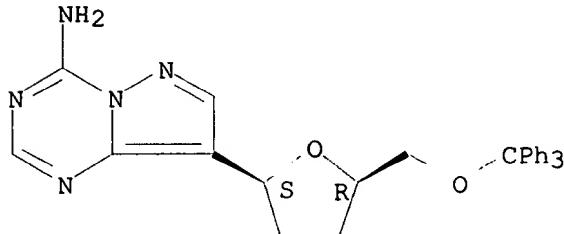
GI



AB 2',3'-Dideoxy-L-C-nucleosides, e.g. I, have been synthesized from L-gulonic .gamma.-lactone.

L17 ANSWER 10 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 179929-57-8 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, 8-[tetrahydro-5-[(triphenylmethoxy)methyl]-2-furanyl]-, (2S-cis)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C29 H27 N5 O2  
 SR CA  
 LC STN Files: CA, CAPLUS

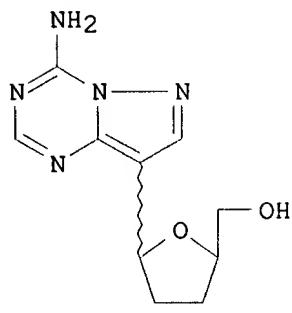
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

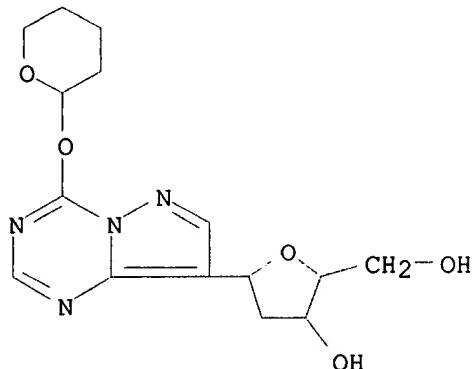
REFERENCE 1: 125:143192 Synthesis of 2',3'-dideoxy-L-glyceropentofuranosyl C-nucleosides. Lee, Chang Soo; Du, Jinfa; Chu, Chung K. (Dep. Med. Chem., Univ. Georgia, Athens, GA, 30602, USA). Nucleosides Nucleotides, 15(6), 1223-1236 (English) 1996.  
 CODEN: NNUUD5. ISSN: 0732-8311.

GI



AB 2',3'-Dideoxy-L-C-nucleosides, e.g. I, have been synthesized from L-gulonic .gamma.-lactone.

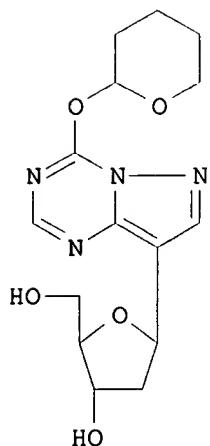
L17 ANSWER 11 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 170717-24-5 REGISTRY  
 CN D-erythro-Pentitol, 1,4-anhydro-2-deoxy-1-C-[4-[(tetrahydro-2H-pyran-2-yl)oxy]pyrazolo[1,5-a]-1,3,5-triazin-8-yl]-, [1R(S)]- (9CI) (CA INDEX NAME)  
 MF C15 H20 N4 O5  
 SR CA  
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

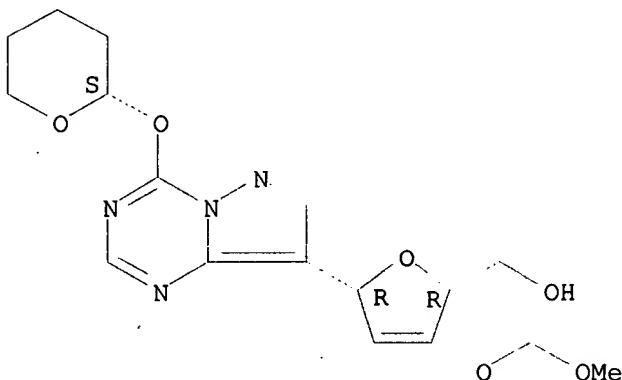
GI



AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prepd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]- 1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of the intermediate silyl enol ether, a C-glycoside analog of adenosine.

L17 ANSWER 12 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 166241-95-8 REGISTRY  
 CN 2-Furanmethanol, 2,5-dihydro-3-(methoxymethoxy)-5-[4-[(tetrahydro-2H-pyran-2-yl)oxy]pyrazolo[1,5-a]-1,3,5-triazin-8-yl]-, [2R-[2.alpha.,5.alpha.(S\*)]]- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C17 H22 N4 O6  
 SR CA  
 LC STN Files: CA, CAPLUS

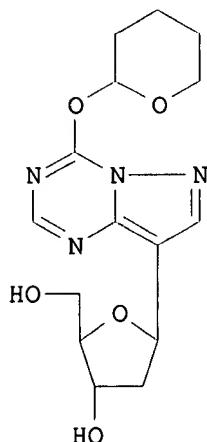
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

GI

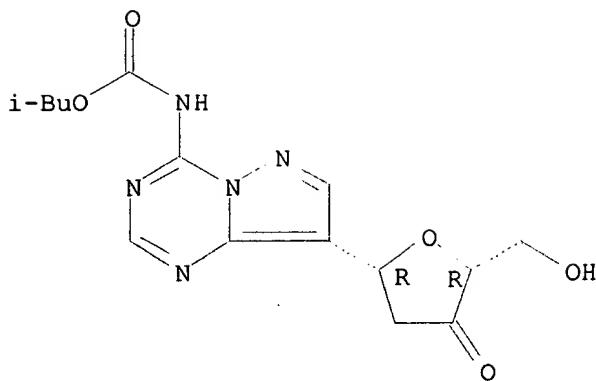


I

AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prepd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]- 1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of the intermediate silyl enol ether, a C-glycoside analog of adenosine.

L17 ANSWER 13 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 162791-81-3 REGISTRY  
CN Carbamic acid, [8-[tetrahydro-5-(hydroxymethyl)-4-oxo-2-furanyl]pyrazolo[1,5-a]-1,3,5-triazin-4-yl]-, 2-methylpropyl ester, (2R-cis)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C15 H19 N5 O5  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

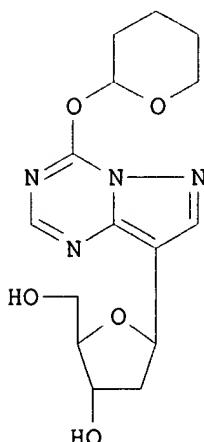
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

GI



I

AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prep'd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]-1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of the intermediate silyl enol ether, a C-glycoside analog of adenosine.

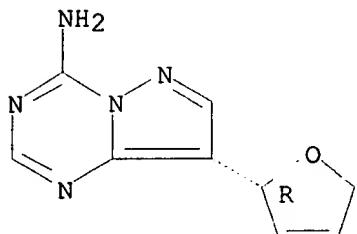
L17 ANSWER 14 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 162791-79-9 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4-amine, 8-(2,5-dihydro-2-furanyl)-,

(R) - (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C9 H9 N5 O  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

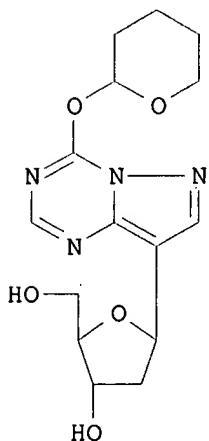
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

GI

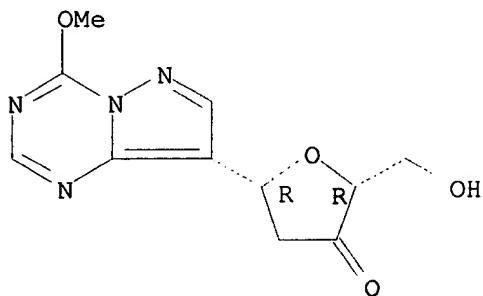


I

AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prep'd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]- 1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of the intermediate silyl enol ether, a C-glycoside analog of adenosine.

RN 162791-76-6 REGISTRY  
 CN 3(2H)-Furanone, dihydro-2-(hydroxymethyl)-5-(4-methoxypyrazolo[1,5-a]-1,3,5-triazin-8-yl)-, (2R-cis) - (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C11 H12 N4 O4  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT

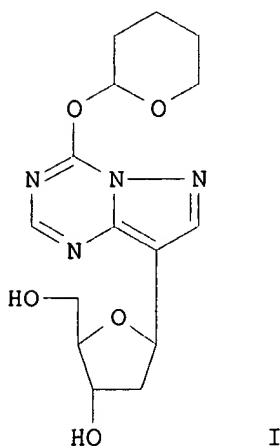
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

GI

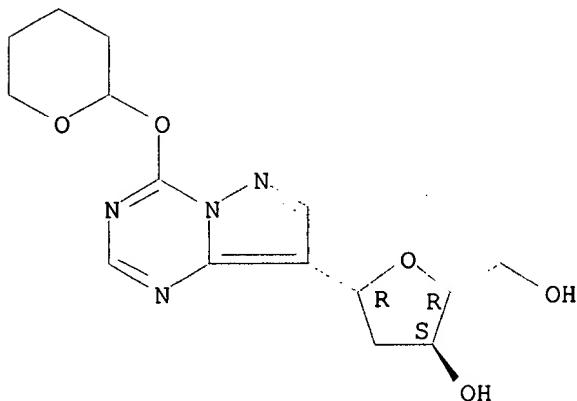


AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prep'd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]-1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of

the intermediate silyl enol ether, a C-glycoside analog of adenosine.

L17 ANSWER 16 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 162791-74-4 REGISTRY  
CN D-erythro-Pentitol, 1,4-anhydro-2-deoxy-1-C-[4-[(tetrahydro-2H-pyran-2-yl)oxy]pyrazolo[1,5-a]-1,3,5-triazin-8-yl]-, [1R(R)]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C15 H20 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

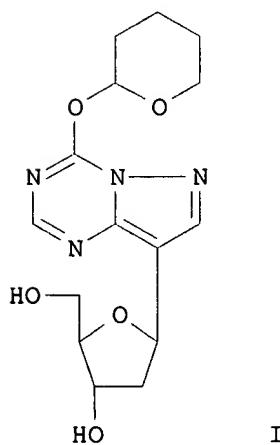
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

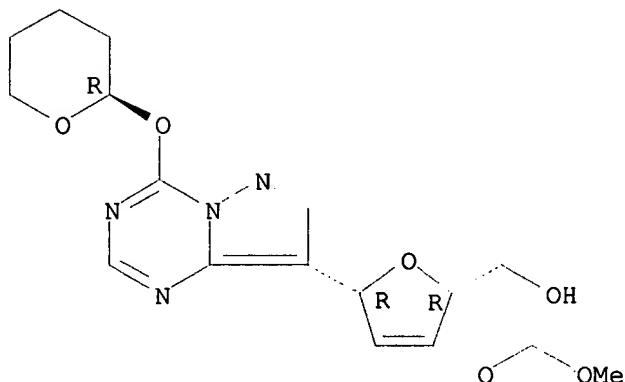
GI



AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prep'd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]- 1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of the intermediate silyl enol ether, a C-glycoside analog of adenosine.

L17 ANSWER 17 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 162791-73-3 REGISTRY  
CN 2-Furanmethanol, 2,5-dihydro-3-(methoxymethoxy)-5-[4-[(tetrahydro-2H-pyran-2-yl)oxy]pyrazolo[1,5-a]-1,3,5-triazin-8-yl]-, [2R-[2.alpha.,5.alpha.(R\*)]]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C17 H22 N4 O6  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

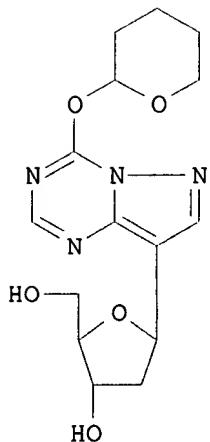
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:291417 Palladium-mediated coupling reactions of an amino-substituted heterocycle. Direct synthesis of C-nucleosides related to adenosine. Zhang, Han-Cheng; Brakta, Mohamed; Davies, G. Doyle, Jr. (Department Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA). Nucleosides Nucleotides, 14(1 & 2), 105-16 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

GI



AB C-nucleosides of the pyrazolo[1,5-a]-1,3,5-triazine aglycon system, e.g. I, have been prepd. by palladium-mediated coupling of 8-iodopyrazolo[1,5-a]-1,3,5-triazines. 4-(N,N'-diisobutyloxycarbonyl)amino-8-iodopyrazolo[1,5-a]- 1,3,5-triazine and the furanoid glycal 1,4-anhydro-2-deoxy-3-O-[(1,1-dimethylethyl)diphenylsilyl]-D-erythro-pent-1-enitol coupled in the presence of catalytic palladium(0) to yield, after desilylation of the intermediate silyl enol ether, a C-glycoside analog of adenosine.

L17 ANSWER 18 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 149065-45-2 REGISTRY

CN D-erythro-Pent-1-enitol, 1,4-anhydro-2-deoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-1-C-[4-[(tetrahydro-2H-pyran-2-yl)oxy]pyrazolo[1,5-a]-1,3,5-triazin-8-yl]- (9CI) (CA INDEX NAME)

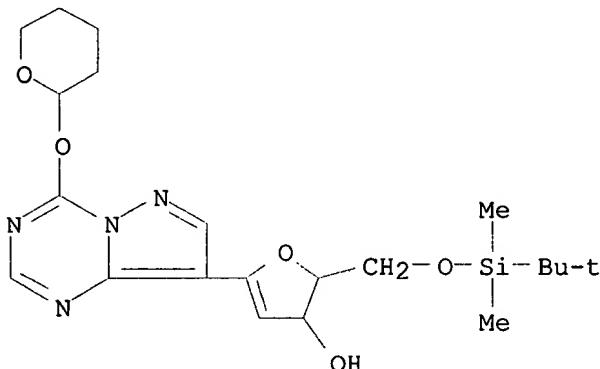
OTHER CA INDEX NAMES:

CN Pyrazolo[1,5-a]-1,3,5-triazine, D-erythro-pent-1-enitol deriv.

MF C21 H32 N4 O5 Si

SR CA

LC STN Files: CA, CAPLUS, CASREACT



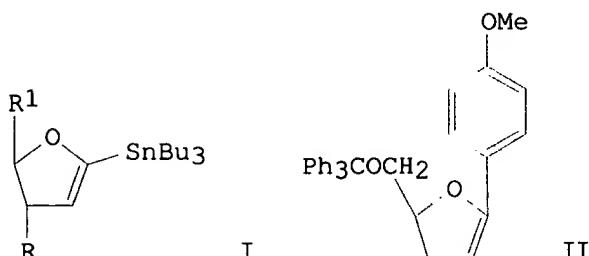
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:117625 Preparation of 1-(tri-n-butylstannylyl) furanoid

glycals and their use in palladium-mediated coupling reactions.  
 Zhang, Han Cheng; Brakta, Mohamed; Daves, G. Doyle, Jr. (Dep. Chem.,  
 Rensselaer Polytech. Inst., Troy, NY, 12180, USA). Tetrahedron  
 Lett., 34(10), 1571-4 (English) 1993. CODEN: TELEAY. ISSN:  
 0040-4039.

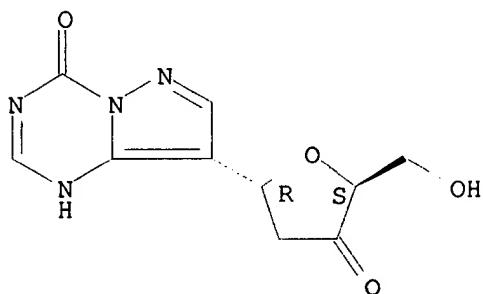
GI



AB 1-(Tri-n-butylstannylyl)furanoid glycals, e.g. I (R = R1 = H; R = OH, R1 = CH2OH; R = H, R1 = CH2OCPH3), have been prepd. for the first time by lithiation of the corresponding 3-O-unsubstituted glycals followed by reaction with tri-n-butylstannylyl chloride. Furanoid glycals bearing an alkoxy (silyloxy) group at C-3 undergo elimination and furan formation. Compds. I underwent palladium-mediated coupling with aryl iodide to yield the corresponding 1-substituted furanoid glycals, e.g. II, in good to excellent yields.

L17 ANSWER 19 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 147976-36-1 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-[tetrahydro-5-(hydroxymethyl)-4-oxo-2-furanyl]-, (2R-trans)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H10 N4 O4  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:9095 Water facilitation of palladium-mediated coupling reactions. Zhang, Han Cheng; Daves, G. Doyle, Jr. (Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180, USA).

Organometallics, 12(5), 1499-500 (English) 1993. CODEN: ORGND7.  
ISSN: 0276-7333.

AB Water-contg. solvent systems are more effective than conventionally used org. reaction solvents for palladium-mediated coupling reactions of iodo derivs. of nitrogen heterocycles with cyclic enol ethers(2,3-dihydrofuran) and furanoid glycals.

L17 ANSWER 20 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 147916-96-9 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-[2,5-dihydro-5-(hydroxymethyl)-4-(methoxymethoxy)-2-furanyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

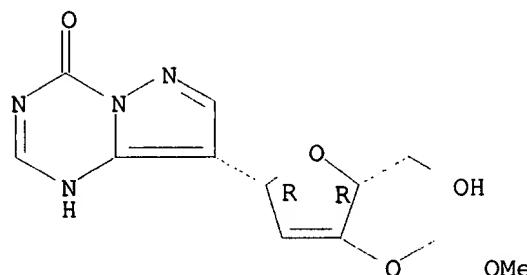
FS STEREOSEARCH

MF C12 H14 N4 O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMINFORMRX

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:9095 Water facilitation of palladium-mediated coupling reactions. Zhang, Han Cheng; Daves, G. Doyle, Jr. (Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180, USA). Organometallics, 12(5), 1499-500 (English) 1993. CODEN: ORGND7. ISSN: 0276-7333.

AB Water-contg. solvent systems are more effective than conventionally used org. reaction solvents for palladium-mediated coupling reactions of iodo derivs. of nitrogen heterocycles with cyclic enol ethers(2,3-dihydrofuran) and furanoid glycals.

L17 ANSWER 21 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 147916-95-8 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-[tetrahydro-5-(hydroxymethyl)-4-oxo-2-furanyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

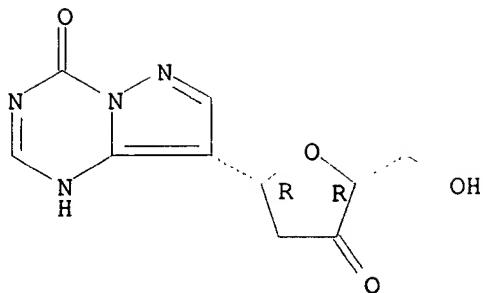
FS STEREOSEARCH

MF C10 H10 N4 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

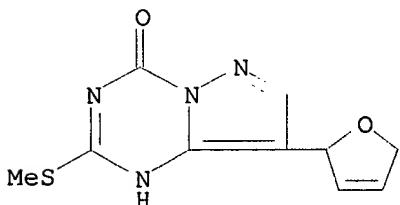


1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:9095 Water facilitation of palladium-mediated coupling reactions. Zhang, Han Cheng; Daves, G. Doyle, Jr. (Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180, USA). Organometallics, 12(5), 1499-500 (English) 1993. CODEN: ORGND7. ISSN: 0276-7333.

AB Water-contg. solvent systems are more effective than conventionally used org. reaction solvents for palladium-mediated coupling reactions of iodo derivs. of nitrogen heterocycles with cyclic enol ethers(2,3-dihydrofuran) and furanoid glycals.

L17 ANSWER 22 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 147916-93-6 REGISTRY  
CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-(2,5-dihydro-2-furanyl)-2-(methylthio)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C10 H10 N4 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT



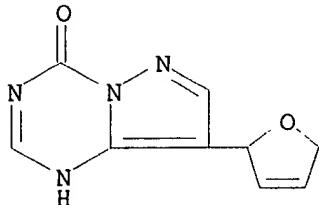
1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:9095 Water facilitation of palladium-mediated coupling reactions. Zhang, Han Cheng; Daves, G. Doyle, Jr. (Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180, USA). Organometallics, 12(5), 1499-500 (English) 1993. CODEN: ORGND7. ISSN: 0276-7333.

AB Water-contg. solvent systems are more effective than conventionally used org. reaction solvents for palladium-mediated coupling reactions of iodo derivs. of nitrogen heterocycles with cyclic enol ethers(2,3-dihydrofuran) and furanoid glycals.

L17 ANSWER 23 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 147916-92-5 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-(2,5-dihydro-2-furanyl)-  
     (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C9 H8 N4 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, CHEMINFORMRX



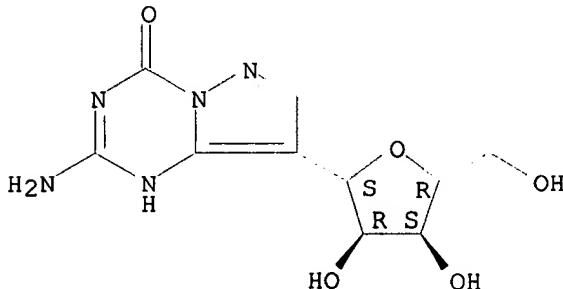
1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:9095 Water facilitation of palladium-mediated coupling reactions. Zhang, Han Cheng; Daves, G. Doyle, Jr. (Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180, USA). Organometallics, 12(5), 1499-500 (English) 1993. CODEN: ORGND7.  
 ISSN: 0276-7333.

AB Water-contg. solvent systems are more effective than conventionally used org. reaction solvents for palladium-mediated coupling reactions of iodo derivs. of nitrogen heterocycles with cyclic enol ethers(2,3-dihydrofuran) and furanoid glycals.

L17 ANSWER 24 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 71774-74-8 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 2-amino-8-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H13 N5 O5  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
     (\*File contains numerically searchable property data)

Absolute stereochemistry.

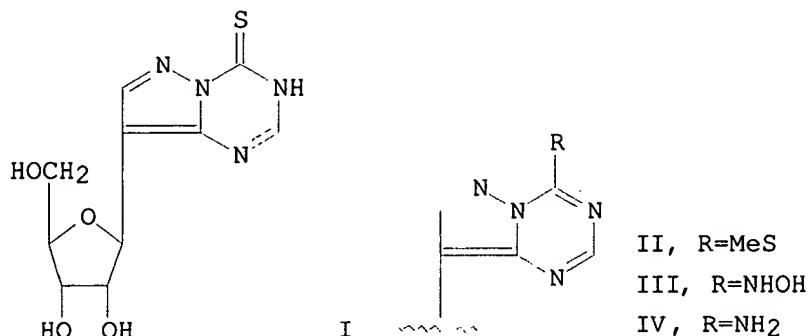


1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve

Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH<sub>2</sub> group of IV with H<sub>2</sub>S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

L17 ANSWER 25 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 71774-73-7 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 2-amino-8-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.beta.-D-ribofuranosyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

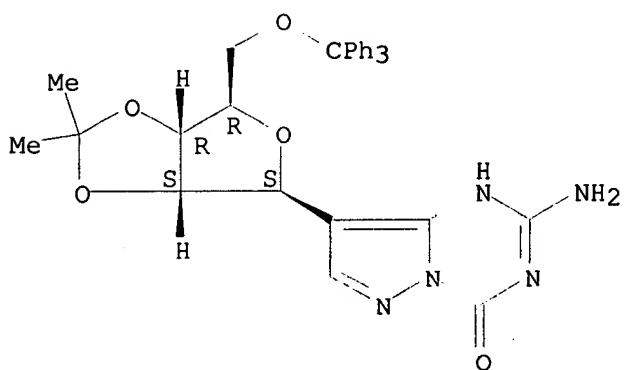
CN Furo[3,4-d]-1,3-dioxole, pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one deriv.

FS STEREOSEARCH

MF C32 H31 N5 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Absolute stereochemistry.

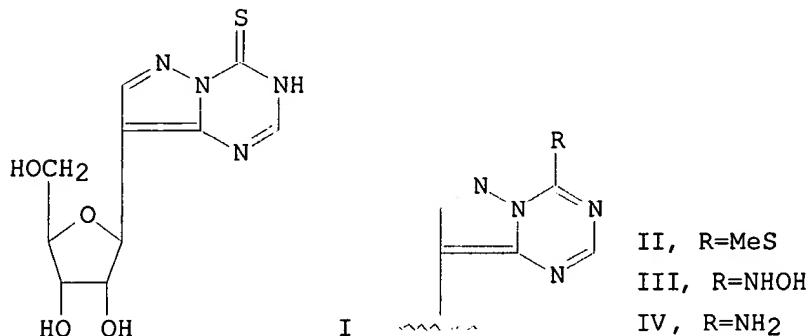


1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

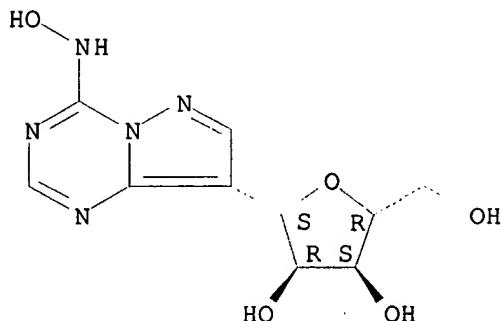
GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH<sub>2</sub> group of IV with H<sub>2</sub>S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

L17 ANSWER 26 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 71774-70-4 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-.beta.-D-ribofuranosyl-, oxime (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H13 N5 O5  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)

Absolute stereochemistry.

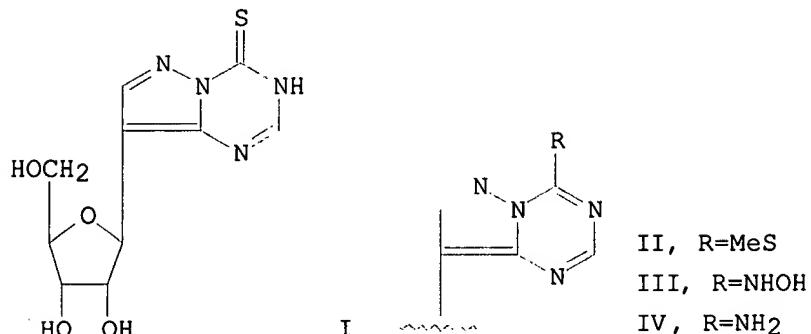


1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med.

Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH<sub>2</sub> group of IV with H<sub>2</sub>S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

L17 ANSWER 27 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 62196-67-2 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.alpha.-D-ribofuranosyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one deriv.

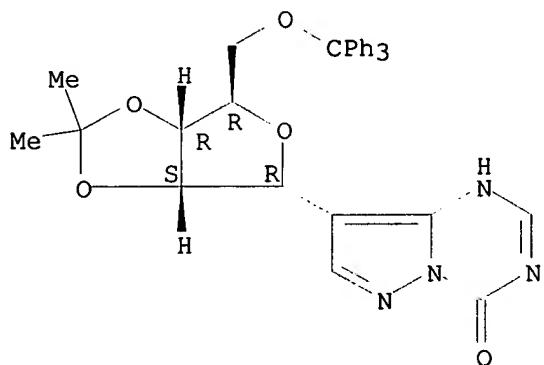
FS STEREOSEARCH

MF C32 H30 N4 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172950 Ring transformation reactions of

C-nucleosides: facile synthesis of pyrazolo[1,5-a]pyrimidine and pyrazolo[1,5-a]triazine C-nucleosides. Chu, C. K.; Suh, J. J.; Mesbah, M.; Cutler, S. J. (Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). J. Heterocycl. Chem., 23(2), 349-52 (English) 1986.  
CODEN: JHTCAD. ISSN: 0022-152X.

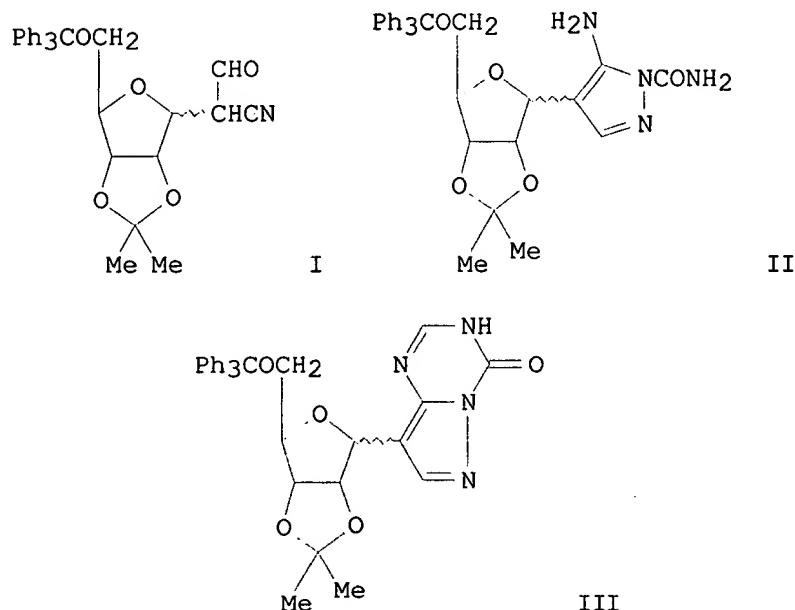
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 1,3-Dimethyluracil (I), a versatile synthon for the synthesis of various heterocycles, reacted readily with 3-aminopyrazoles II in sodium ethoxide to give pyrazolo[1,5-a]pyrimidines III. Under similar conditions, 3-aminopyrazole C-nucleosides IV and the synthon I gave a mixt. of pyrazolo[1,5-a]pyrimidine C-nucleosides, which was sepd. on a silica gel column. Attempts to remove the protecting groups yielded pyranose deriv. V. Another synthon 1,3-dimethyl-5-azauracil and 3-aminopyrazoles gave pyrazolo[1,5-a]triazines. In a similar reaction IV gave the corresponding pyrazolo[1,5-a]triazine C-nucleoside VI and its .alpha.-anomer.

REFERENCE 2: 95:7661 Nucleosides. 117. Synthesis of 4-oxo-8-(.beta.-D-ribofuranosyl)-3H-pyrazolo[1,5-a]-1,3,5-triazine (OPTR) via 3-amino-2N-carbamoyl-4-(.beta.-D-ribofuranosyl)pyrazole (ACPR) derivatives. Chu, C. K.; Watanabe, K. A.; Fox, J. J. (Mem. Sloan-Kettering Cancer Cent., Sloan-Kettering Inst., New York, NY, 10021, USA). J. Heterocycl. Chem., 17(7), 1435-9 (English) 1980.  
CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Reaction of ribofuranosylacetonitrile (I) with semicarbazide hydrochloride followed by NaOEt treatment afforded an

.alpha., .beta.-mixt. of ribofuranosylpyrazole II. Conversion of II to ribofuranosylpyrazolotriazine (III) was achieved by treatment of II with HC(OEt)<sub>3</sub>. The .beta.-isomer II gave only the .beta.-isomer III, and the .alpha.-isomer was converted exclusively into the .alpha.-isomer III. Upon deprotection with 3% BuOH-HCl, both II gave the same mixt. of the .alpha.- and .beta.-isomers of 3-amino-2-N-carbamoyl-4-(D-ribosyl)pyrazole, which were sepd. by chromatog. The syntheses of the hitherto unknown compds., 3-amino-2-N-carbamoylpyrazole and its 4-Me analog are also reported. Exptl. details of the synthesis of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole, an important intermediate for purine-like C-nucleosides, are also described.

REFERENCE 3: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOET and EtO<sub>2</sub>CN:CHOET with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

L17 ANSWER 28 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 62156-22-3 REGISTRY

CN D-Ribitol, 1-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-1,4-anhydro-2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-, (R)-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, D-ribitol deriv.

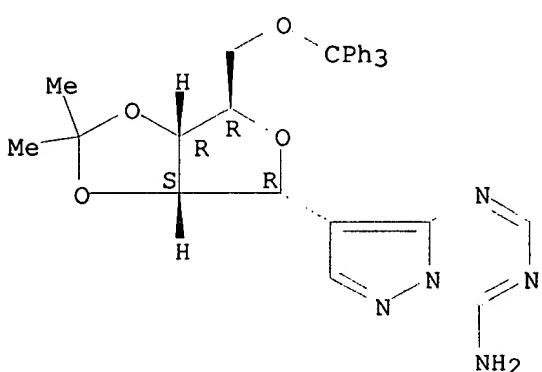
CN Pyrazolo[1,5-a]-1,3,5-triazine, D-ribitol deriv.

FS STEREOSEARCH

MF C32 H31 N5 O4

LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Absolute stereochemistry.



2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 101:38762 Synthesis of 3-amino-2-carbamimidoylpyrazole C-nucleosides and its cyclization to 4-aminopyrazolo[1,5-a]-1,3,5-triazine C-nucleosides. Chu, Chung K. (Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). Heterocycles, 22(2), 345-51 (English) 1984. CODEN: HTCYAM. ISSN: 0385-5414.

AB 4-Amino-8-(.beta.-D-2,3-O-isopropylidene-5-O-tritylribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine and its .alpha.-isomer were synthesized from 2-formyl-2-(2,3-O-isopropylidene-5-O-trityl-D-ribofuranosyl)acetonitrile and aminoguanidine nitrate via 3-amino-2-carbamimidoyl-4-(.alpha. and .beta.-D-2,3-O-isopropylidene-5-O-tritylribofuranosyl)pyrazoles.

REFERENCE 2: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOET and EtO<sub>2</sub>CN:CHOET with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

L17 ANSWER 29 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 62156-21-2 REGISTRY

CN D-Ribitol, 1-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-1,4-anhydro-, (R)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

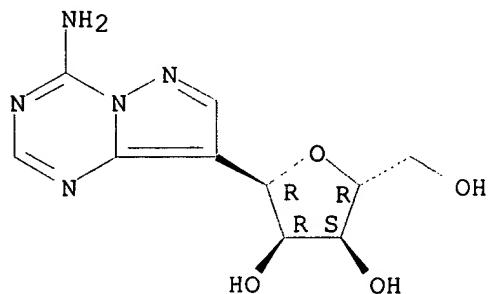
CN Pyrazolo[1,5-a]-1,3,5-triazine, D-ribitol deriv.

FS STEREOSEARCH

MF C10 H13 N5 O4

LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Absolute stereochemistry.



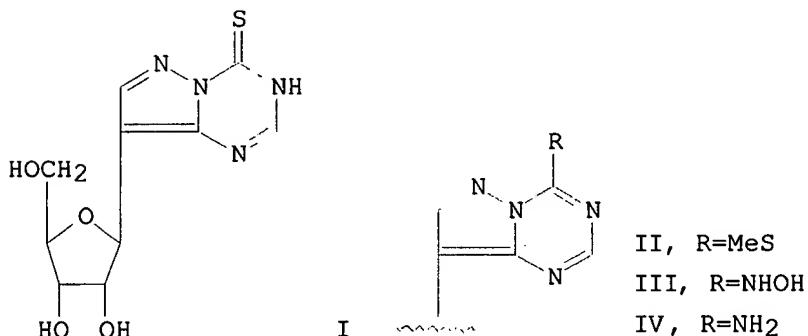
2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:6862 Nucleosides. 112. Synthesis of some new

pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH<sub>2</sub> group of IV with H<sub>2</sub>S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

REFERENCE 2: 86:121673 Nucleosides. CV. Synthesis of the  
 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres  
 of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las  
 Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst.,  
 Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6),  
 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

Treatment of NCN:CHOET and Eto2CN:CHOEt with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary *in vitro* antileukemia testing results of I are included.

L17 ANSWER 30 OF 37 REGISTRY COPYRIGHT 1998 ACS

BN 62156-20-1 REGISTRY

KN 32150-20-1 RECBIRI  
CN D-Ribitol, 1-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-1,4-anhydro-2,3-O-(1-methylethyldene)-5-O-(triphenylmethyl)-, (S)-(9CI) (CA INDEX NAME)

**OTHER CA INDEX NAMES:**

CN Furo[3,4-d]-1,3-dioxole, D-ribitol deriv.

CN Pyrazolo[1,5-a]-1,3,5-triazine, D-ribitol deriv.

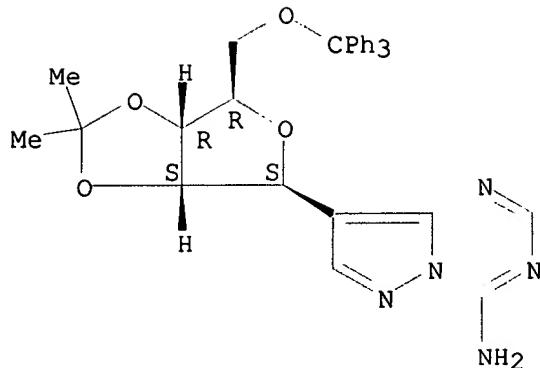
ES STEREOSEARCH

STEREOSEARCH  
C32 H31 N5 O4

LC STN Files: BEILSTEIN\* CA CAPIUS

LC SIN Files. BEILENSTein, CA, CAFLOS  
(\*File contains numerically searchable property data)

## Absolute stereochemistry.



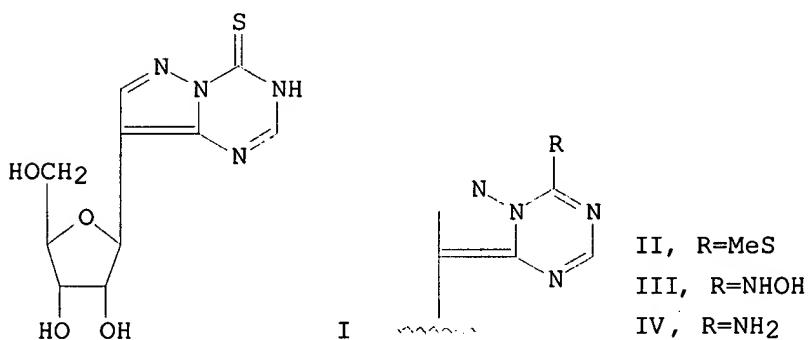
3 REFERENCES IN FILE CA (1967 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 101:38762 Synthesis of 3-amino-2-carbamimidoylpyrazole C-nucleosides and its cyclization to 4-aminopyrazolo[1,5-a]-1,3,5-triazine C-nucleosides. Chu, Chung K. (Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). Heterocycles, 22(2), 345-51 (English) 1984. CODEN: HTCYAM. ISSN: 0385-5414.

AB 4-Amino-8-(.beta.-D-2,3-O-isopropylidene-5-O-tritylribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine and its .alpha.-isomer were synthesized from 2-formyl-2-(2,3-O-isopropylidene-5-O-trityl-D-ribosyl)acetonitrile and aminoguanidine nitrate via 3-amino-2-carbamimidoyl-4-(.alpha. and .beta.-D-2,3-O-isopropylidene-5-O-tritylribofuranosyl)pyrazoles.

REFERENCE 2: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH2 group of IV with H2S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

REFERENCE 3: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOET and EtO<sub>2</sub>CN:CHOEt with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

L17 ANSWER 31 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 62156-19-8 REGISTRY

CN D-Ribitol, 1-C-(4-aminopyrazolo[1,5-a]-1,3,5-triazin-8-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

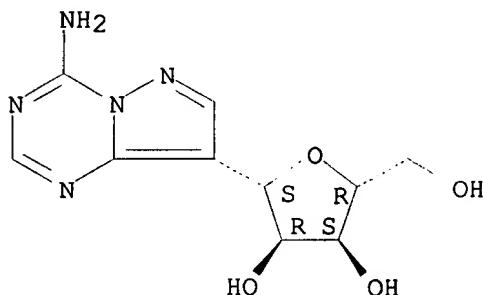
CN Pyrazolo[1,5-a]-1,3,5-triazine, D-ribitol deriv.

FS STEREOSEARCH

MF C10 H13 N5 O4

LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Absolute stereochemistry.

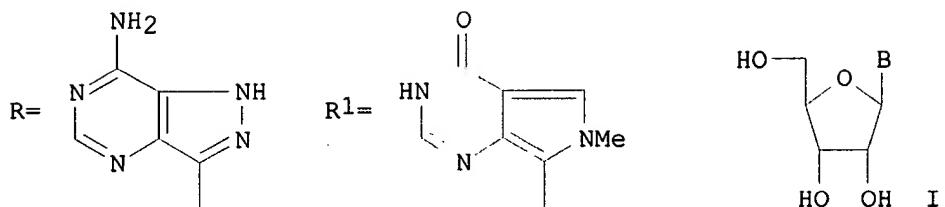


4 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:290158 Conformational properties of purine-like C-nucleosides. Otter, Brian A.; Klein, Robert S. (Dep. of Oncology, Montefiore Medical Center, Bronx, NY, 10467, USA). Nucleosides Nucleotides, 15(1-3), 793-807 (English) 1996. CODEN: NUNUD5. ISSN: 0732-8311.

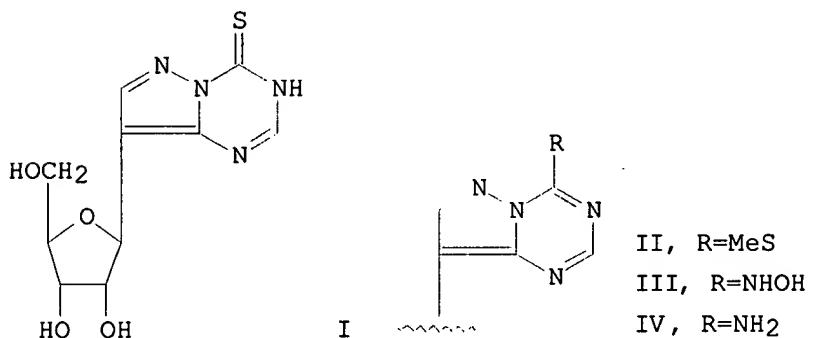
GI



AB The multiplicities and chem. shifts of the 5'-hydroxyl resonances in the NMR spectra of a series of purine-like C-nucleosides, e.g. I (B = R, R1), reflect the presence of a hydrogen bond to N(1), and hence afford a method for assessing soln. syn/anti conformational preferences.

REFERENCE 2: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH<sub>2</sub> group of IV with H<sub>2</sub>S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

REFERENCE 3: 91:15775 Adenosine kinase from rabbit liver. II. Substrate and inhibitor specificity. Miller, Richard L.; Adamczyk, David L.; Miller, Wayne H.; Koszalka, George W.; Rideout, Janet L.; Beacham, Lowrie M., III; Chao, Esther Y.; Haggerty, Jerald J.; Krenitsky, Thomas A.; Elion, Gertrude B. (Wellcome Res. Lab., Research Triangle Park, NC, 27709, USA). J. Biol. Chem., 254(7), 2346-52 (English) 1979. CODEN: JBCHA3. ISSN: 0021-9258.

AB Kinetic consts. for substrates and inhibitors of highly purified rabbit liver adenosine kinase were detd. for 119 nucleosides and nucleoside analogs. The enzyme was relatively nonsp. with regard to the base moiety of ribonucleosides. The best substrates were adenosine, 8-azaadenosine, toyocamycin, and sangivamycin. Although imidazole ribonucleosides and some of their analogs served as substrates, their K'm values were >1000 times that of adenosine.

None of the pyrimidine ribonucleosides tested were substrates or inhibitors. The enzyme was relatively specific for the ribosyl moiety. 2'-Deoxyadenosine and arabinosyladenine were extremely poor substrates, with substrate efficiencies of 10-4-10-6 that of adenosine. Binding of the inhibitor, 5'-deoxy-5'-aminoadenosine appeared to be pH-dependent. Basically, these results support the suggestion that a 2'-hydroxyl group trans to the glycoside linkage is a prerequisite for substrate activity or appreciable binding to the enzyme. A trans-2'-amino group was able to replace the 2'-hydroxyl group without loss of substrate activity. Studies with adenosine analogs locked in defined conformations suggest that binding to the enzyme does not appear to be solely dependent upon conformation.

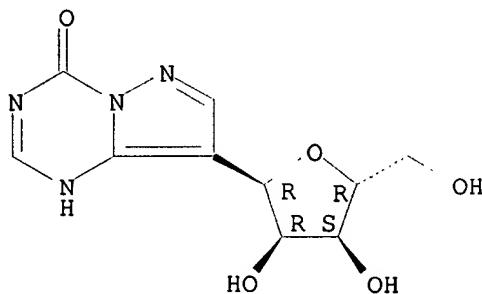
REFERENCE 4: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOET and EtO2CN:CHOET with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

L17 ANSWER 32 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 62156-08-5 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-.alpha.-D-ribofuranosyl- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H12 N4 O5  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)

Absolute stereochemistry.

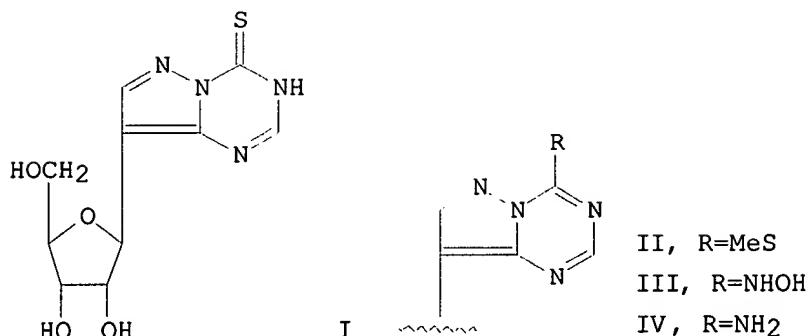


2 REFERENCES IN FILE CA (1967 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med.

Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH<sub>2</sub> group of IV with H<sub>2</sub>S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

REFERENCE 2: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOEt and EtO<sub>2</sub>CN:CHOEt with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

L17 ANSWER 33 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 62156-07-4 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.beta.-D-ribofuranosyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

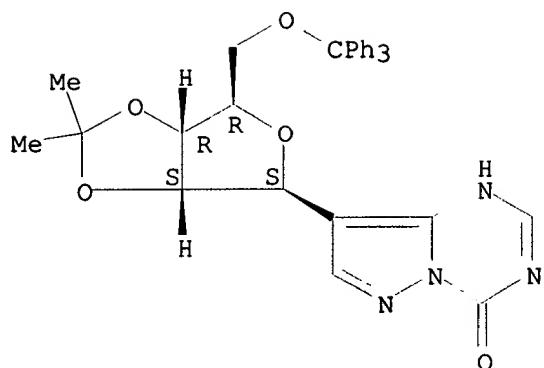
CN Furo[3,4-d]-1,3-dioxole, pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one deriv.

FS STEREOSEARCH

MF C32 H30 N4 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172950 Ring transformation reactions of C-nucleosides: facile synthesis of pyrazolo[1,5-a]pyrimidine and pyrazolo[1,5-a]triazine C-nucleosides. Chu, C. K.; Suh, J. J.; Mesbah, M.; Cutler, S. J. (Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA). J. Heterocycl. Chem., 23(2), 349-52 (English) 1986.  
CODEN: JHTCAD. ISSN: 0022-152X.

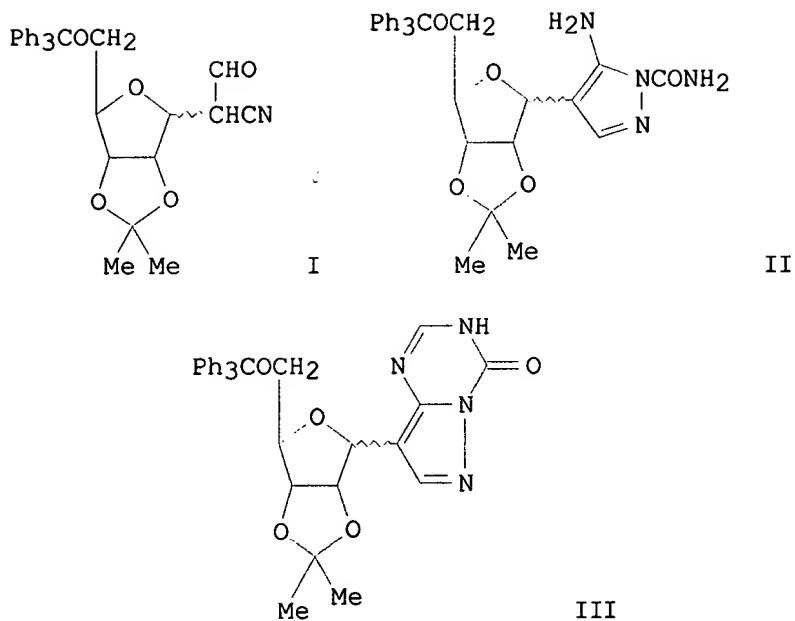
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 1,3-Dimethyluracil (I), a versatile synthon for the synthesis of various heterocycles, reacted readily with 3-aminopyrazoles II in sodium ethoxide to give pyrazolo[1,5-a]pyrimidines III. Under similar conditions, 3-aminopyrazole C-nucleosides IV and the synthon I gave a mixt. of pyrazolo[1,5-a]pyrimidine C-nucleosides, which was sepd. on a silica gel column. Attempts to remove the protecting groups yielded pyranose deriv. V. Another synthon 1,3-dimethyl-5-azauracil and 3-aminopyrazoles gave pyrazolo[1,5-a]triazines. In a similar reaction IV gave the corresponding pyrazolo[1,5-a]triazine C-nucleoside VI and its .alpha.-anomer.

REFERENCE 2: 95:7661 Nucleosides. 117. Synthesis of 4-oxo-8-(.beta.-D-ribofuranosyl)-3H-pyrazolo[1,5-a]-1,3,5-triazine (OPTR) via 3-amino-2N-carbamoyl-4-(.beta.-D-ribofuranosyl)pyrazole (ACPR) derivatives. Chu, C. K.; Watanabe, K. A.; Fox, J. J. (Mem. Sloan-Kettering Cancer Cent., Sloan-Kettering Inst., New York, NY, 10021, USA). J. Heterocycl. Chem., 17(7), 1435-9 (English) 1980.  
CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Reaction of ribofuranosylacetonitrile (I) with semicarbazide hydrochloride followed by NaOEt treatment afforded an .alpha.,.beta.-mixt. of ribofuranosylpyrazole II. Conversion of II to ribofuranosylpyrazolo[1,5-a]-1,3,5-triazine (III) was achieved by treatment of II with HC(OEt)<sub>3</sub>. The .beta.-isomer II gave only the .beta.-isomer III, and the .alpha.-isomer was converted exclusively into the .alpha.-isomer III. Upon deprotection with 3% BuOH-HCl, both II gave the same mixt. of the .alpha.- and .beta.-isomers of 3-amino-2N-carbamoyl-4-(D-ribosyl)pyrazole, which were sepd. by chromatog. The syntheses of the hitherto unknown compds., 3-amino-2-N-carbamoylpyrazole and its 4-Me analog are also reported. Exptl. details of the synthesis of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole, an important intermediate for purine-like C-nucleosides, are also described.

REFERENCE 3: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOET and EtO<sub>2</sub>CN:CHOET with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

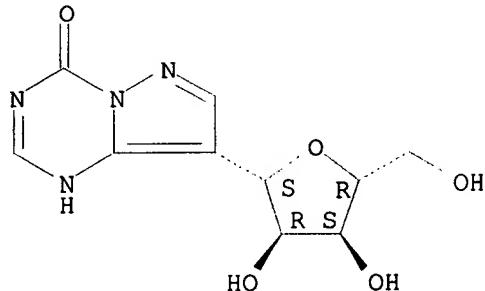
L17 ANSWER 34 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 62156-06-3 REGISTRY

CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 8-.beta.-D-ribofuranosyl-

(9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C10 H12 N4 O5  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)

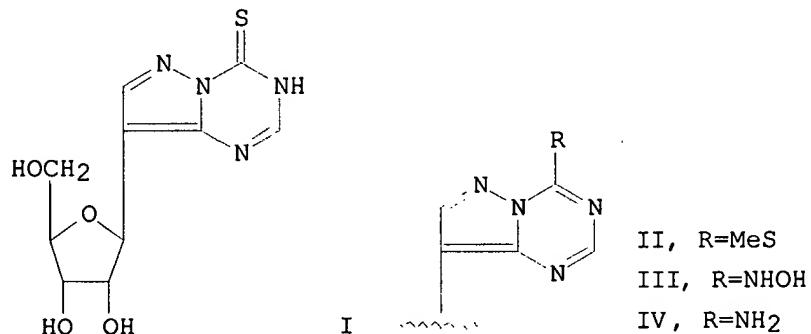
Absolute stereochemistry.



2 REFERENCES IN FILE CA (1967 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:6862 Nucleosides. 112. Synthesis of some new pyrazolo[1,5-a]-1,3,5-triazines and their C-nucleosides. Tam, Steve Y. K.; Klein, Robert S.; Wempen, Iris; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, NY, 10021, USA). J. Org. Chem., 44(25), 4547-53 (English) 1979. CODEN: JOCEAH. ISSN: 0022-3263.

GI



AB The synthesis of pyrazolotriazine C-nucleosides I, II, and III is described. A key step in the conversion IV .fwdarw. I .fwdarw. II .fwdarw. III involves direct substitution of the 4-NH2 group of IV with H2S. The .beta. configuration at C-1' is retained throughout this sequence. Synthesis of the corresponding and as yet unknown pyrazolotriazine bases is also described.

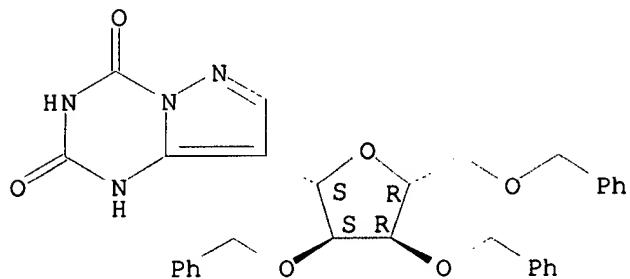
REFERENCE 2: 86:121673 Nucleosides. CV. Synthesis of the 8-(.beta.-D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine isosteres of adenosine and inosine. Tam, S. Y. K.; Hwang, J. S.; De las Heras, F. G.; Klein, R. S.; Fox, J. J. (Sloan-Kettering Inst., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(6), 1305-8 (English) 1976. CODEN: JHTCAD.

GI For diagram(s), see printed CA Issue.

AB Treatment of NCN:CHOET and EtO<sub>2</sub>CN:CHOEt with 3-aminopyrazole gave 4-amino- and 4-oxo-3H-pyrazolo[1,5-a]-1,3,5-triazine, resp. Reaction of 3-amino-4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)pyrazole with the same reagents gave the blocked 4-amino-8-ribosyl- and 4-oxo-3H-8-ribosylpyrazolo[1,5-a]-1,3,5-triazine, resp., deblocking of which in acid gave I and II. The corresponding derivs. in the .alpha.-series were made by identical procedures for confirming all structural assignments. Preliminary in vitro antileukemia testing results of I are included.

L17 ANSWER 35 OF 37 REGISTRY COPYRIGHT 1998 ACS  
RN 59464-09-4 REGISTRY  
CN Pyrazolo[1,5-a]-1,3,5-triazine-2,4(1H,3H)-dione,  
8-[2,3,5-tris-O-(phenylmethyl)-.beta.-D-ribofuranosyl]- (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C31 H30 N4 O6  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, SPECINFO  
(\*File contains numerically searchable property data)

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

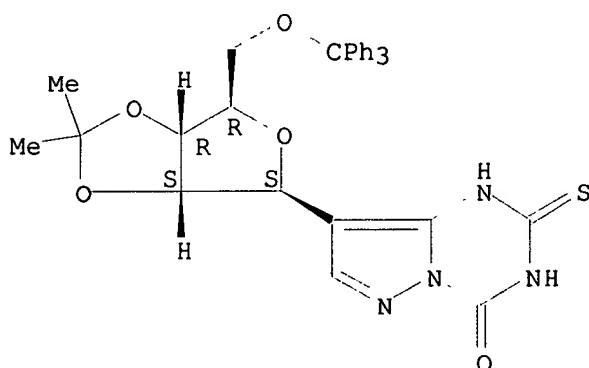
REFERENCE 1: 85:108920 C-glycosyl nucleosides. 9. An approach to the synthesis of purine-related C-glycosides. Gupta, Chhitar M.; Jones, Gordon H.; Moffatt, John G. (Inst. Mol. Biol., Syntex Res., Palo Alto, Calif., USA). J. Org. Chem., 41(18), 3000-9 (English) 1976.  
CODEN: JOCEAH.

AB The synthesis of 4-(2,3,5-tri-O-benzyl-.beta.-D-ribofuranosyl)-3(5)-carbomethoxypyrazole (I) was investigated. The 2,5-anhydro-3,4,6-tri-O-benzyl-D-allose was converted to the C-glycosyl acrylate II via a Wittig reaction followed by cycloaddn. of CH<sub>2</sub>N<sub>2</sub> and dehydrogenation with chlorine. Alternatively I was prep'd. via cycloaddn. of CH<sub>2</sub>N<sub>2</sub> to Me 3-(2,3,5-tri-O-benzyl-.beta.-D-ribofuranosyl)propionate (III). Condensation of 2,3,5-tri-O-benzyl-D-ribose with a Grignard reagent derived from propionic acid gave, after esterification, 5,6,8-tri-O-benzyl-2,3-dideoxy-D-altro-oct-2-ynonate (IV), which with CH<sub>2</sub>N<sub>2</sub> followed by acid-catalyzed cyclization gave I. Although acid-catalyzed cyclization of IV was unsuccessful, reaction with Me(PhO)<sub>3</sub>P-I gave III. The pyrazole ester I was converted into a 3-aminopyrazole via a Curtius reaction on the acyl azide. Cyclization with phenoxy carbonyl isocyanate followed by debenylation with BC<sub>13</sub> gave the purine-related C-glycoside 2,4-dioxo-8-.beta.-D-ribofuranosyl-1H,3H-pyrazolo[1,5-a]-1,3,5-triazine.

L17 ANSWER 36 OF 37 REGISTRY COPYRIGHT 1998 ACS

RN 59414-68-5 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 2,3-dihydro-8-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.beta.-D-ribofuranosyl]-2-thioxo- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Furo[3,4-d]-1,3-dioxole, pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one deriv.  
 FS STEREOSEARCH  
 MF C32 H30 N4 O5 S  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)

Absolute stereochemistry.

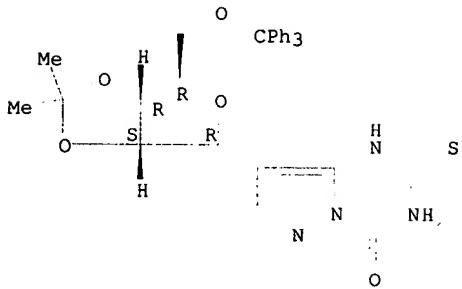


1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 84:180522 Nucleosides. XCVII. Synthesis of an 8-(D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine. A new type of C-nucleoside. De las Heras, Federico G.; Chu, Chung K.; Tam, Steve Y. K.; Klein, Robert S.; Watanabe, Kyoichi A.; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(1), 175-7 (English) 1976. CODEN: JHTCAD.  
 GI For diagram(s), see printed CA Issue.  
 AB Hydrolysis of I (R = CO<sub>2</sub>Et), prep'd. from Me 4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)-1H-pyrazole-5-carboxylate, with NaOH gave 21.5% I (R = H) (II) and 40% of its .alpha.-anomer (III) by epimerization. Treatment of IV (R = CH<sub>2</sub>CN) with HCO<sub>2</sub>Et and NaOEt in anhydrous ether gave IV [R = C(CN):CHONa] which reacted with MeI and cyclized with N<sub>2</sub>H<sub>4</sub> in the presence of NaOEt to give 12% II and 18% III. II and III reacted with SCNCO<sub>2</sub>Et in MeCN and cyclized to give V and its .alpha.-anomer, resp.

L17 ANSWER 37 OF 37 REGISTRY COPYRIGHT 1998 ACS  
 RN 59221-03-3 REGISTRY  
 CN Pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one, 2,3-dihydro-8-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.alpha.-D-ribofuranosyl]-2-thioxo- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Furo[3,4-d]-1,3-dioxole, pyrazolo[1,5-a]-1,3,5-triazin-4(1H)-one deriv.  
 FS STEREOSEARCH  
 MF C32 H30 N4 O5 S  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

- REFERENCE 1: 84:180522 Nucleosides. XCVII. Synthesis of an 8-(D-ribofuranosyl)pyrazolo[1,5-a]-1,3,5-triazine. A new type of C-nucleoside. De las Heras, Federico G.; Chu, Chung K.; Tam, Steve Y. K.; Klein, Robert S.; Watanabe, Kyoichi A.; Fox, Jack J. (Grad. Sch. Med. Sci., Cornell Univ., New York, N. Y., USA). J. Heterocycl. Chem., 13(1), 175-7 (English) 1976. CODEN: JHTCAD.  
GI For diagram(s), see printed CA Issue.  
AB Hydrolysis of I (R = CO<sub>2</sub>E<sub>t</sub>), prep'd. from Me 4-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)-1H-pyrazole-5-carboxylate, with NaOH gave 21.5% I (R = H) (II) and 40% of its .alpha.-anomer (III) by epimerization. Treatment of IV (R = CH<sub>2</sub>CN) with HCO<sub>2</sub>E<sub>t</sub> and NaOEt in anhydrous ether gave IV [R = C(CN):CHONa] which reacted with MeI and cyclized with N<sub>2</sub>H<sub>4</sub> in the presence of NaOEt to give 12% II and 18% III. II and III reacted with SCNCO<sub>2</sub>E<sub>t</sub> in MeCN and cyclized to give V and its .alpha.-anomer, resp.

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